Introduction to the Materials Science of

Rechargeable Batteries

Week 1: Basic Concepts, Fundamentals, and Definitions
Lecture 1.5: Week 1 Summary

By R. Edwin Garcia
Associate Professor of Materials Engineering
Purdue University
A Sketch of a Rechargeable Battery

\[ S_z A \rightleftharpoons zS^+ + A + ze^- \]

\[ S_z A \rightleftharpoons zS + A \]

- (-) \( S_z A \) \quad (electrolyte) \quad (+) \( S_z C \)

\[ zS \rightarrow ze \]

\[ zS + C \rightleftharpoons S_z C \]

\[ zS^+ + C + ze^- \rightleftharpoons S_z C \]
Potential of Electrodes

Anode Potential:

\[ S_z A \rightleftharpoons zS^+ + A + ze^- \]

\[ \varphi_A = \frac{\Delta G_f^A}{zF} : \text{voltage of anode} \]

Cathode Potential:

\[ zS^+ + C + ze^- \rightleftharpoons S_z C \]

\[ \varphi_C : \text{voltage of cathode} \]

Cell Potential:

\[ \Delta \varphi = \varphi_C - \varphi_A \]
Battery Charge

For Each Phase

\[ Q = z \times C_T \times V \times eN_a \]

- **valence**
- **solubility limit**
- **volume of electrode**

For the Device

\[ Q = A \int_{t_0}^{t_f} I \, dt \]

- electronic charge
- Avogadro’s Number
- Faraday’s constant

Units: mA h
Electrode Materials

Porous Battery Capacity

For the Entire Device

\[ Q_c = z F c^c_T (1 - \epsilon_c - \epsilon_f) h_c \]

\[ Q_a = z F c^a_T (1 - \epsilon_a - \epsilon_f) h_a \]

Capacity Ratio

\[ R_c = \frac{Q_c}{Q_a} = \frac{c^c_T (1 - \epsilon_c - \epsilon_f) h_c}{c^a_T (1 - \epsilon_a - \epsilon_f) h_a} \]

Units:

- \( Q_c \): mA h/m^2
- \( Q_a \): dimensionless
- \( R_c \): dimensionless
Energy and Energy Density

\[ U = \frac{\int_{t_0}^{t_f} I(t)E(t)dt}{M_t} \]

For a composite battery:

\[ U = \frac{QE_{ideal}}{M_t} = \min\{Q_c, Q_a\} \frac{E_{ideal}}{W_t} \]

\[ = \frac{E_c - E_a}{W_t} zF c_T^i (1 - \epsilon_i - \epsilon_f) h_i \]
Power and Power Density

\[
P = \frac{\int_{t_\circ}^{t_f} I(t) E(t) dt}{(t_f - t_\circ) M_t}
\]

For a composite battery:

\[
P = \frac{Q E_{\text{ideal}}}{W_t(t_f - t_\circ)} = \min\{Q_c, Q_a\} \frac{E_{\text{ideal}}}{W_t(t_f - t_\circ)}
\]

\[
= \frac{E_c - E_a}{W_t(t_f - t_\circ)} z F c_T^i (1 - \epsilon_i - \epsilon_f) h_i
\]
Ragone Plot